

Spurious localized highest-frequency modes in Schrödinger-type equations solved by finite-difference methods

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Abstract

High-frequency solutions of one or several Schrödinger-type equations are well known to differ very little from the plane wave solutions $\exp[\pm ikx]$. That is, the potential terms impact the envelope of a high-frequency plane wave by only a small amount. However, when such equations are solved by a finite-difference method, the highest-frequency solutions may, under certain conditions, turn out to be localized. In this letter we explain this numerical artifact.

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Coupled Schrödinger-type equations arise in many areas of physics, e.g., in quantum mechanics [1, 2, 3, 4] and stability of nonlinear waves [5]. Often, the problem is posed as an eigenvalue problem whereby localized eigenfunctions and their eigenvalues are sought. The eigenfunction localization occurs due to the presence of potential-like terms. A simple approach of solving such an eigenvalue problem is to discretize the equations by a finite-difference method and then solve the resulting matrix eigenvalue problem by a commercial software. Then, by inspection or otherwise, one selects the localized eigenfunctions and their eigenvalues out of a set of eigensolutions produced by the software.

High-frequency solutions are, typically, not sought numerically because their approximate analytical form can be found by perturbation methods, e.g., by the Born or Wentzel–Kramers–Brillouin approximations. For example, for a single Schrödinger equation

$$-d^2\psi/dx^2 + V(x)\psi = \lambda\psi, \quad \lambda > 0, \quad (1)$$

where $\lambda \gg 1$ and $V(x)$ varies on the scale of order one and also $\max |V(x)| = O(1)$, the latter approximation yields:

$$\psi(x) = \left(\frac{\lambda}{\lambda - V(x)} \right)^{1/4} \exp \left[\pm i \left\{ \sqrt{\lambda} x - \frac{1}{\sqrt{\lambda}} \int V(x) dx \right\} \right] \left(1 + O \left(\frac{1}{\sqrt{\lambda}} \right) \right). \quad (2)$$

Moreover, to accurately resolve a solution with a given frequency, one needs about 10 grid points per wavelength. The highest-frequency mode resolved on a grid with a step size h has a wavelength $2h$; that is, such a mode has only 2 grid points per wavelength. Thus, one does not expect that such a mode can be resolved with much quantitative accuracy. However, one does expect that it should qualitatively look like solution (2): its envelope is to be a finite constant away from the localized potential $V(x)$ and is to have a small “wiggle” around the potential.

The researcher may want to inspect the numerically obtained highest-frequency solutions of the eigenproblem in order to verify that at least in the high-frequency limit, his/her finite-difference code produces reasonable results, as described above. If the code produces *qualitatively* different profiles of high-frequency modes, the researcher may question the correctness of the code and search for a mistake. This can be a time-consuming task when a system of several coupled equations is considered. Thus, it is valuable to know what the highest-frequency modes obtained by a finite-difference method can look like.

Below we show that such modes look not at all as described at the end of the paragraph containing Eq. (2). Rather, their envelopes are the *lowest*-frequency eigenfunctions of the potential $-V(x)$. In short, this occurs because the finite-difference approximation to d^2/dx^2 in (1) evaluated on the highest-frequency carrier $\exp[ikx]$ with $k = \pi/h$ becomes “const $-d^2/dx^2$ ”; note the change of sign in front of the second derivative. Observing localized envelopes of the numerically obtained highest-frequency modes may be even more counterintuitive given that they occur for a repulsive rather than attractive potential.

While we noticed this fact when numerically solving several coupled Schrödinger-type equations, below we chose to present its explanation for a single equation (1), so that the complexity of the problem would not obfuscate the essence of the explanation. As a finite-difference approximation of $d^2\psi/dx^2$ we use the simple central difference:

$$d^2\psi(x_n)/dx^2 \approx (\psi(x_{n+1}) - 2\psi(x_n) + \psi(x_{n-1}))/h^2, \quad (3)$$

where $x_{n\pm 1} = x_n \pm h$. Using a more accurate Numerov's discretization [2] leads to the same qualitative conclusions.

The following Matlab code computes the four highest-frequency modes and the corresponding eigenvalues of Eq. (1) with $V(x) = 3 \operatorname{sech}(0.5x)$ and periodic boundary conditions:

```
h=0.1; x=-16:h:16-h; N=length(x);
M=spdiags(repmat([-1 2 -1],N,1),[-1 0 1],N,N)/h^2 + diag(3*sech(0.5*x));
M(1,end)=-1/h^2; M(end,1)=-1/h^2;
[Evecs, Evals]=eigs(M,4,'lm'); absEvecs=abs(Evecs);
k=1; plot(x,sech(0.5*x),'--',x,absEvecs(:,k)/max(absEvecs(:,k))));
```

The envelopes of the first and fourth such modes are shown in Figs. 1(a,b); the carrier is shown in Fig. 1(c). As we have announced above, these envelopes are localized, in contrast to the slightly perturbed plane waves (2) that could have been expected naively. A calculation that explains Fig. 1 is as follows.

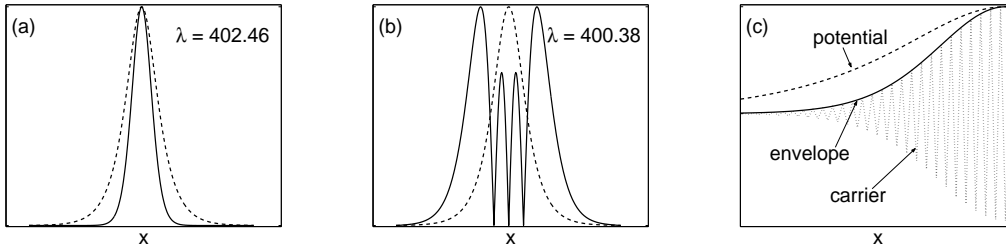


Figure 1: (a,b) Solid lines show envelopes of the first and fourth highest-frequency modes obtained by the finite-difference approximation of (1) with $V = 3 \operatorname{sech}(0.5x)$. Dashed line show the potential $V(x)$. The corresponding eigenvalues are shown in each panel. (c) Part of panel (a), magnified and displaying the highest-frequency carrier.

As Fig. 1(c) illustrates, one can take $\psi(x_n) = \exp[i\pi n] \phi(x_n)$. Here the factor $\exp[i(\pi/h)x_n] = \exp[i\pi n]$ accounts for the highest-frequency carrier, while $\phi(x_n)$ is assumed to vary on the x -scale of order one. Substituting this ansatz into (1) where the second derivative is approximated by (3), one finds:

$$\frac{4}{h^2}\phi(x) + \frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) + O(h^2) = \lambda\phi. \quad (4)$$

Here $x \equiv x_n$, and we have used the Taylor expansion $\phi(x_{n\pm 1}) = \phi(x) \pm h\phi'(x) + (h^2/2)\phi''(x) + O(h^3)$ for the smooth envelope $\phi(x)$. Neglecting the $O(h^2)$ -term in (4), one sees that that

equation becomes

$$\phi'' + (V - \Delta\lambda)\phi = 0, \quad \Delta\lambda = \lambda - (4/h^2). \quad (5)$$

Based on (5), one can make the following conclusions about the appearance of the envelopes of the high-frequency modes of (1) obtained by a finite-difference approximation. When the potential in the original Eq. (1) is repulsive, $V(x) > 0$ (or, more generally, $\int_{-\infty}^{\infty} V(x) dx > 0$), the envelope of the mode with the highest eigenvalue λ is the ground state of (5). For smaller λ 's, one obtains consecutive excited states of (5). This is confirmed by Fig. 1(a,b). The taller and/or wider the potential, the more high-frequency modes with localized envelopes there exist. The non-localized envelopes, corresponding to $\Delta\lambda < 0$ is (5), still have spatial features on the scale of order one (see Fig. 2(a)). For an attractive potential in (1), $V(x) < 0$, there exist no localized solutions of (5). In that case, the envelopes of all high-frequency modes are not localized. Such envelopes of the first and fifth highest-frequency modes for $V(x) = -3 \operatorname{sech}(0.5x)$ are shown in Fig. 2(b,c).

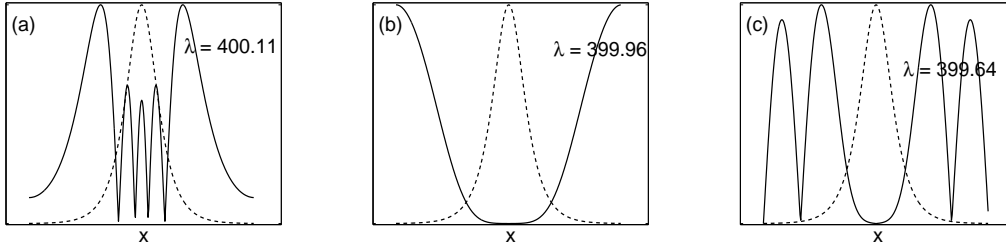


Figure 2: As in Fig. 1, solid and dashed lines show the moduli of the mode envelope and of the potential. (a) The fifth (non-localized) highest-frequency mode obtained by the finite-difference approximation of (1) with $V = 3 \operatorname{sech}(0.5x)$. (b,c) First and fourth highest-frequency modes (non-localized) for the potential $V = -3 \operatorname{sech}(0.5x)$.

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